Thermal Stability Investigation using Ellipsometry

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Outline

- Introduction – Replacement of the JFTOT color standard
- Methods – Principles of Ellipsometry
- Results – Discussion of repeatability, increasing temperature, and increasing naphthalene concentration
- Conclusion

Introduction – Thermal Stability

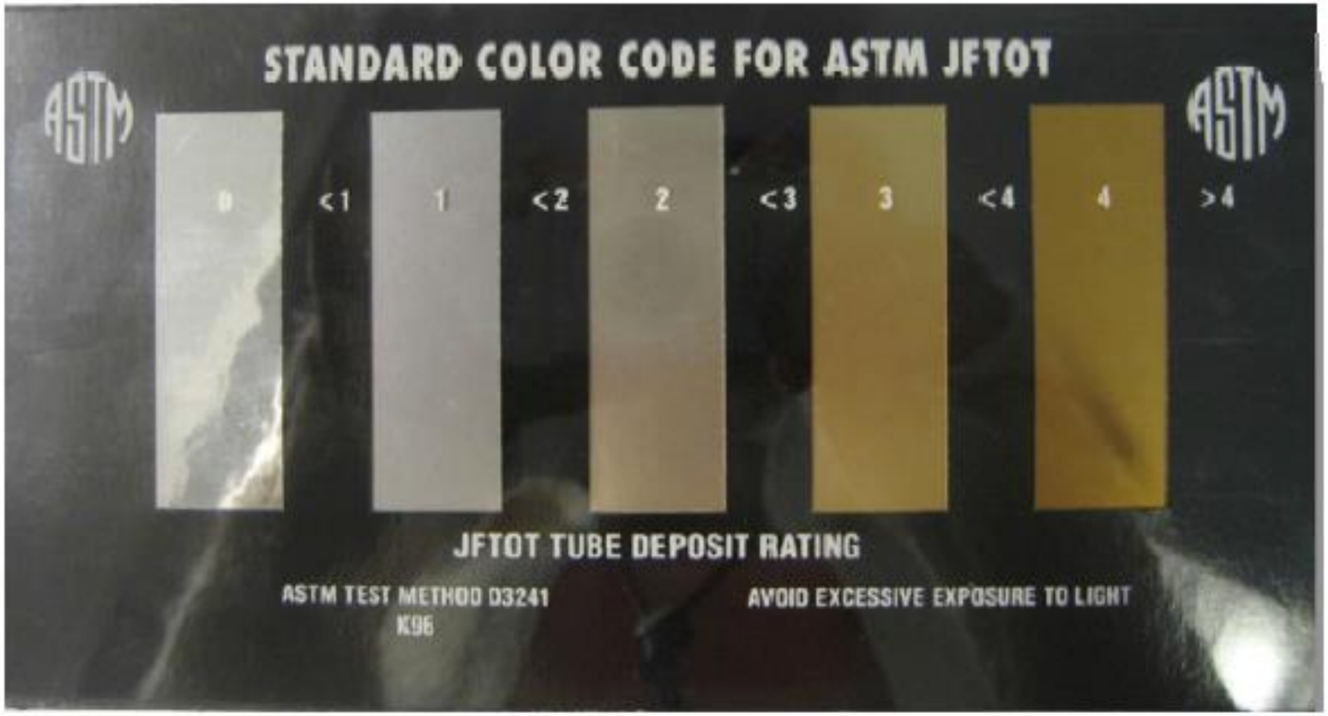
- Defined as the degree to which a fuel breaks down when heated
- Poor thermal stability leads to engine component fouling and decreased fuel flow
- Important to understand to anticipate maintenance schedules and component wear

Introduction – Jet Fuel Thermal Oxidation Test

- ASTM Standard D3241 “Standard Test Method for Thermal Oxidation Stability of Aviation Turbine Fuels”
  - Resistively heat tubes to 260 °C
  - Flow fuel for 2.5 hours
  - Perform color and pressure tests
  - Increase temperature by 5 °C and repeat until failure

Introduction – Jet Fuel Thermal Oxidation Test

- Color standard



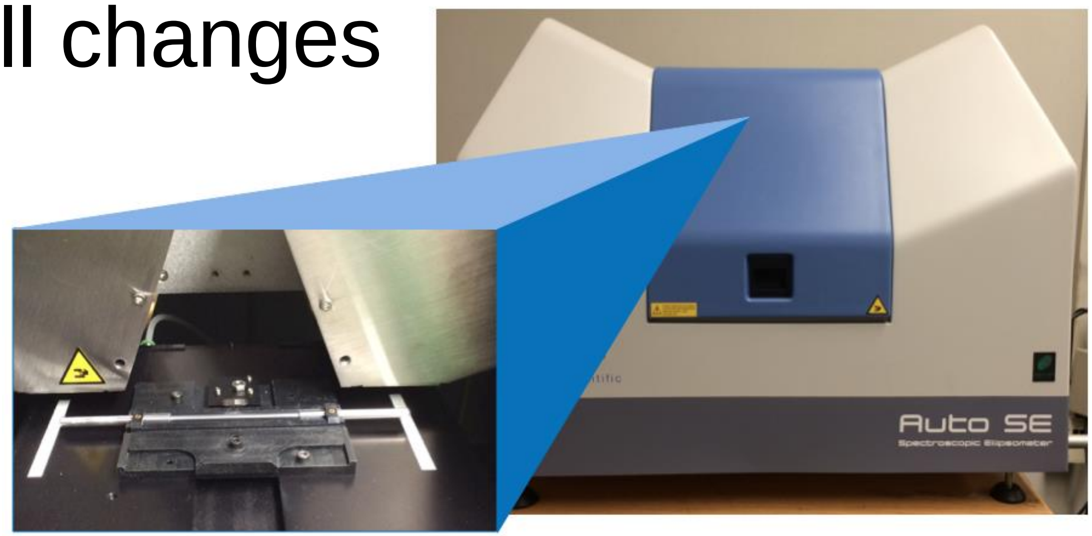
Browne, S. T., Wong, H., Hinderer, C. B., and Klettlinger, J. "Enhancement of Aviation Fuel Thermal Stability Characterization Through Application of Ellipsometry," 2012.

- 3 or greater is failing

Introduction – Implementation of Ellipsometry

- Ellipsometry added to ASTM D3241

- Benefits
  - –Quantitative
  - –Sensitive to small changes
  - –Nondestructive
  - –Versatile



Introduction – Sasol IPK and Naphthalene

- Sasol Iso-Paraffinic Kerosene: Fisher-Tropsch synthetic jet fuel

–Mostly C_{10} and C_{12} isoparaffins (>95%)

–Far fewer components than traditional jet fuels

- Naphthalene: 2 ringed aromatic additive

Introduction – Fuel Composition

Fuel	Aromatics v%	Mercaptan Sulfur m%	Total Sulfur m%	Hydrogen Content m%
Sasol IPK	0.5	<0.001	<0.001	15.1
S-8	0.0	0.000	0.002	15.4
Jet A	18.7	0.001	0.21	14.09
JP-8	16.5	0.000	0.060	13.8

Moses, C. A. "Comparative evaluation of semi-synthetic jet fuels," *Contract* Vol. 33415, No. 02-D, 2008, p. 229

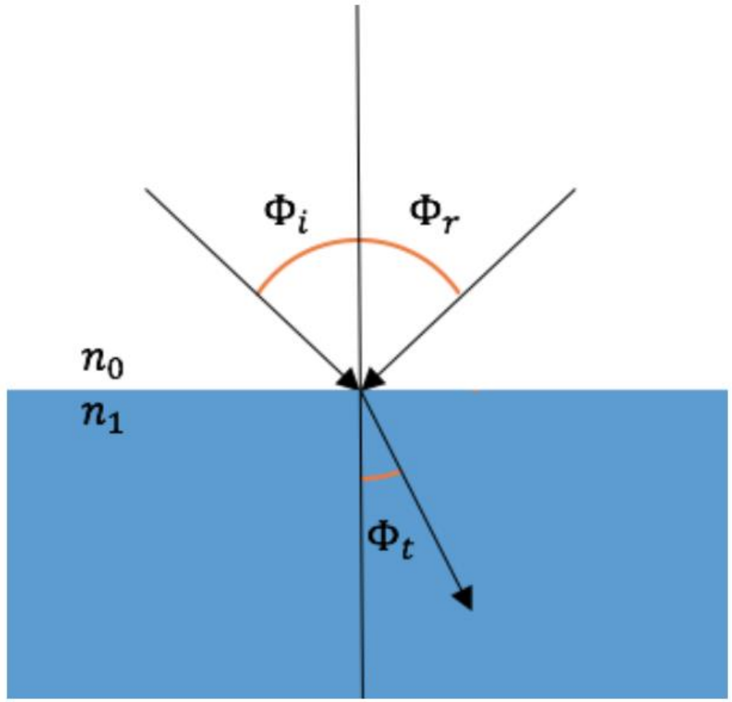
Methods – Tube Preparation with HLPS

- Tubes prepared with Hot Liquid Process Simulator

- Used JFTOT specifications except for tube substrate

Methods – Principles of Ellipsometry

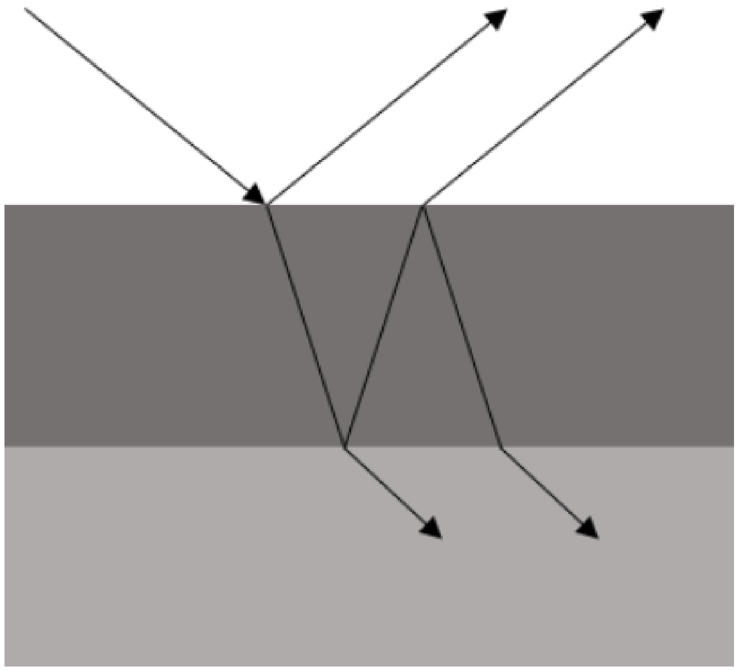
- At an interface light reflects and refracts according to Snell's Law



$$n_0 \sin(\phi_i) = n_1 sin(\phi_1)$$

Methods – Principles of Ellipsometry

- Reflection and refraction occurs at each interface



Methods – Principles of Ellipsometry

- Fresnel Relations used to track intensity and phase through each interface and calculates thickness

$$R^p = \frac{r_{12}{}^p + r_{23}{}^p \exp(-j2\beta)}{1 + r_{12}{}^p r_{23}{}^p \exp(-j2\beta)}$$

$$R^s = \frac{r_{12}{}^s + r_{23}{}^s \exp(-j2\beta)}{1 + r_{12}{}^s r_{23}{}^s \exp(-j2\beta)}$$

Methods – Modeling

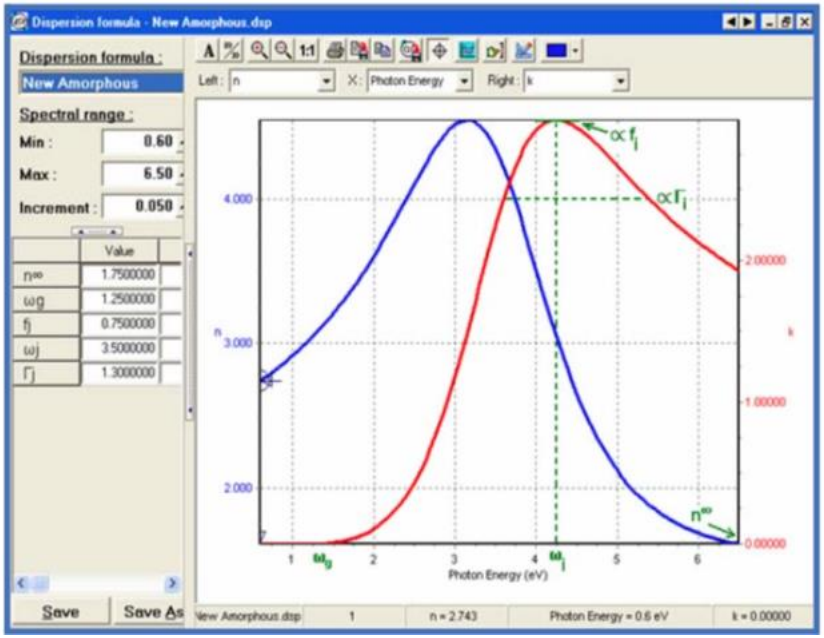
- New amorphous dispersion formula used to model n and k change with wavelength

$$k(\omega) = \sum_{j=1}^{N} \frac{f_j(\omega - \omega_g)^2}{(\omega - \omega_j)^2 + \Gamma_j^2} \; for \; \omega > \omega_g \qquad n(\omega) = n_\infty + \sum_{j=1}^{N} \frac{B_j(\omega - \omega_j) + C_j}{(\omega - \omega_j)^2 + \Gamma_j^2}$$

$$k(\omega) = 0 \; for \; \omega \leq \omega_g$$

$$B_j = \frac{f_j}{\Gamma_j}\left[\Gamma_j^2 - (\omega_j - \omega_g)^2\right]$$

$$C_j = 2 f_j \Gamma_j (\omega_j - \omega_g)$$



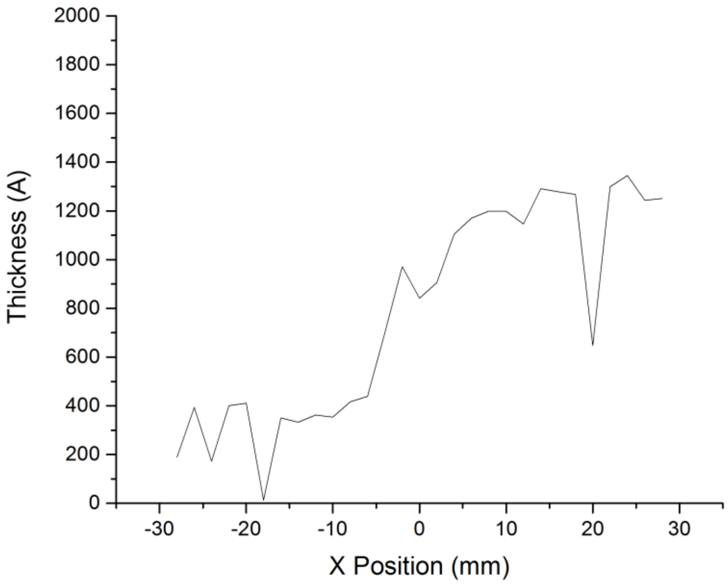
Horiba New Amorphous Dispersion Formula.

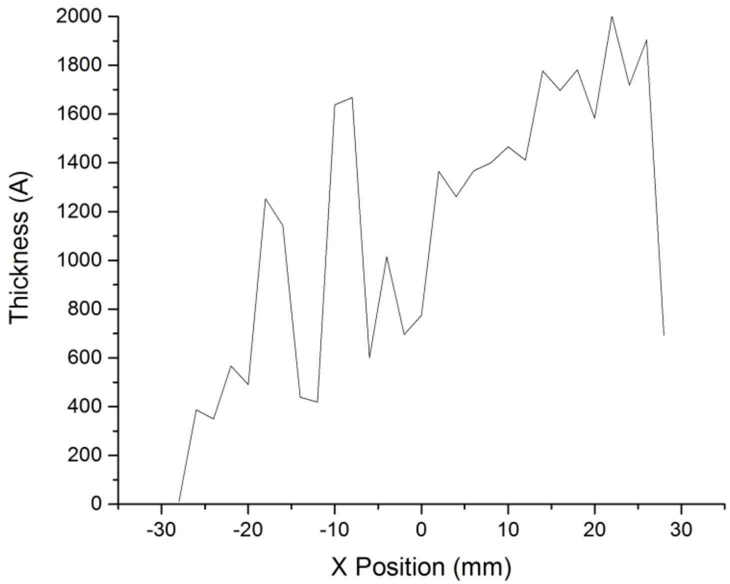
Results – Repeatability

- Tubes 1311 and 1329
  - Sasol IPK with 99% naphthalene
  - 385 K
  - 1334.87 and 1278.22 Å (4.2% difference)

Results – Increasing Temperature

- Deposit thickness increases with increasing temperature





Results – Increasing Naphthalene Concentration

- Increasing naphthalene concentration increases deposit thickness

Tube Number	Temperature (K)	Percent Naphthalene	Average Deposit Thickness (Å)
1309	385	0	1037.438
1329	385	1	1278.222
1332	385	3	1307.806
1333	385	5	1796.44

- Opposite effect seen in aluminum tubes

Future Work

- Measure thermal stability of other fuels and additives using the same technique
- Perform more tests at identical conditions to better asses repeatability
- Create predictive model for deposit thickness

Conclusion

- Ellipsometry has been added to the thermal stability standard
- This method was shown to be repeatable
- Increasing temperature increases the deposit thickness
- Increasing naphthalene concentration increases deposit thickness

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Questions?